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Statistical description of glass network interconnectivity in calcium aluminosilicate glasses

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Two series of peralkaline glasses with a composition close to the eutectic compositions of anorthite-wollatsonite-gehlenite and anorthite-wollasonite-tridymite were synthesized and investigated using ^{29}Si and ^{27}Al MAS-NMR. The structure of the glass is described by a network of $SiO_{4/2}$ and $AlO_{4/2}^-$ tetrahedrons as network former and Ca^{2+} ions as charge compensation for $AlO_{4/2}^-$ or as network modifier. Besides the separation into bridging oxygen and non-bridging oxygen, the 2nd coordination sphere is described by a combinatorial statistic continuous random network or by a hierarchic random network. The description of the network is used to calculate the molar fraction of Si with different first (O) and second (Si or Al) coordination sphere. The ratio of the areas of the ^{29}Si NMR resonances of the different coordinated Si specimens is assumed to be proportional to the molar fraction obtained from the structural models. The other parameters for the peaks attributed to different ^{29}Si specimens are calculated by fitting the measured spectra. The quasi heterogeneous modeling approach with a hierarchy in the intermediate range order results in the best description of the NMR spectra while the intensities obtained from combinatorial statistic continuous random network do not result is a proper fit. This procedure of analyzing common ^{29}Si MAS-NMR gives hints, that the investigated Ca-aluminosilicate glasses are best described by a quasi-heterogeneous intermediate range order.